Benzene

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 93.8 °C

Global applicability domain: Inside

Local applicability domain index: 6.41e-01

Confidence level: 7.49e-01

Nearest Neighbors from the Training Set

Image not found

Benzene
Measured: 80.0
Predicted: 93.8

Image not found

1,3,5-Cycloheptatriene
Measured: 117
Predicted: 112

Image not found

Toluene
Measured: 111
Predicted: 110

Image not found

2,5-Norbornadiene
Measured: 89.5
Predicted: 99.2